

Crystallography News

British Crystallographic Association

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Scenes in Montreal around the IUCr Congress

BCA Spring Meeting, 2015

IUCr Congress in Montreal Reports

Education and Outreach Update

Crystallography Fights Ebola

Crystallography Fights Cancer

p6

p10

p17

p18

p20

Pictures (clockwise) from top left:

- YCs enjoying poutine
- cyclist sign
- acrobats
- Gautam Desiraju
- crystal-like buildings
- poster session

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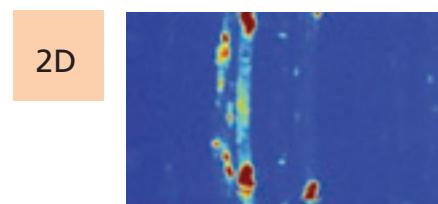
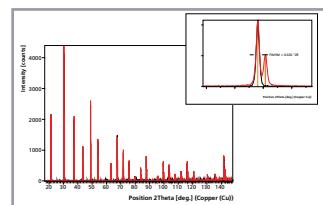
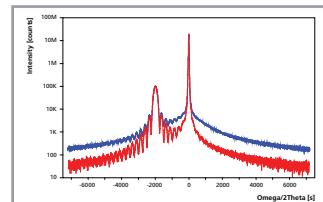


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**BCA Administrative Office,**

First Floor
Hornbeam House
Hornbeam Business Park
Harrogate HG2 8QT
Tel: +44 (0)1423 855 990
Fax: +44 (0)1423 855 999
e-mail: bca@hg3.co.uk

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Carl Schwalbe
15 St Augustine Drive
Droitwich
Worcs WR9 8QR
Tel: 01905 775257
e-mail: carlschwalbe@hotmail.com

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These details are not divulged to any others without your permission. You may inspect your entry during the Annual Meeting, or otherwise by application to the BCA Administrative Office. We will be happy to amend entries at any time.

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Contents

From the President	2
BCA Council 2014	3
From the Editor	4
Puzzle 'Poets' Corner	5
BCA Annual Spring Meeting, 2015	6
The IUCr Congress in Montreal	10
Education and Outreach Update	17
Crystallography Fights Ebola	18
BSG Winter Meeting	19
Using Crystals to Cure Cancer	20
Dr Frank Allen 1944-2014	21
A Crystallographic Dinosaur	22
Book Review	24
Meetings of Interest	25

This month's cover:

Montreal pictures by
Joshua Hill, Joan Schwalbe
and Carl Schwalbe



From the President



RECENTLY I have been spending a lot of time working with the photographer **Max Alexander**, **Claire Murray** and others to prepare for the “Illuminating Atoms” photographic exhibition in the Royal Albert Hall. This exhibition (in the usual time-shifted way that I have to write this column) has been showing throughout November and

includes portraits of crystallographers, many of whom are well known to us, and photographs that document our working environment and methods. The Royal Albert Hall might not be considered a natural location for such an exhibition but – by being freely available to all people coming to any RAH event – it reaches people groups who might not necessarily prioritize visiting a science-based exhibition. Indeed as I write this, the RAH website shows a photograph of crystallographer **Stephen Moggach** alongside the 2014 Statoil Masters Tennis promotion! So if you have been fielding crystallography-related questions from **Jools Holland** fans or the world’s best tennis players and their followers then this exhibition might be why.

As part of our preparations for the event some of us took a trip to the seaside at Porthcawl to replicate a neutron diffraction pattern of quartz on the beach using bulb-planters and seed dibbers. After three or four hours ‘hard work’ on the sand in the sunshine **Sam Callear**, **Anna** and **Mark Warren** and myself had carefully mapped out the required 641 holes for the Laue pattern of quartz looking down the c-axis. I then had to wait for the sun to go in for Max to take my photograph with the pattern while Sam and Mark went swimming – it was a great day out of the office and the locals certainly enjoyed our crazy creation! If you missed the exhibition then I believe that it is also being shown as a slideshow on the STFC website – including the final photo of our seaside scene.

For those of you who managed to get to the IUCr Congress in Montreal in August I hope that you enjoyed it as much as I did. We had a great representation from the UK in the scientific sessions with excellent talks from students and established professors alike. Following voting at the General Assembly in Montreal, the UK is now also strongly represented on the IUCr Executive Committee; congratulations to **Mike Glazer** as the new IUCr Vice President!

By the time you are reading this, the International Year of Crystallography 2014 will be drawing to a close. Looking back on the year, I am delighted with what we have achieved; crystallography has escaped from its traditional scientific confines to reach public awareness through radio programmes (I hope that you managed to catch **Elspeth Garman** on Radio 4’s “The Life Scientific”), online content, public exhibitions, stands at science fairs around the country (we were recently at Grantham’s ‘Gravity Fields’ festival), crystal-growing competitions and general articles in a number of more general-audience journals. This has been possible through the hard work and, at times, tenacity of our members

and I am very pleased with the way that we have collectively grabbed this opportunity to share our subject with those around us. Thank you to BCA Council for providing funds, to our Education and Outreach Co-ordinators for their active co-ordination, to the many volunteers and to those outside the BCA who have supported this work financially and through collaborative projects. I hope that you agree that it has been good fun as well! And you’ll be pleased to know that we plan to continue with a stand at the Big Bang Fair (NEC, 11-14 March) next year as well...

The draft programme for next year’s Spring Meeting in York is in this issue of *Crystallography News*. As you will see, the much-expanded programme has excellent plenary speakers, more scientific sessions and a strand of workshops running throughout the meeting. Please do support this meeting, by registering to attend, offering to contribute talks and posters and encouraging others to do the same. The Programme Organising Committee are working hard to give you an excellent and rewarding meeting – and you’ll also have an opportunity to vote for your next BCA President!

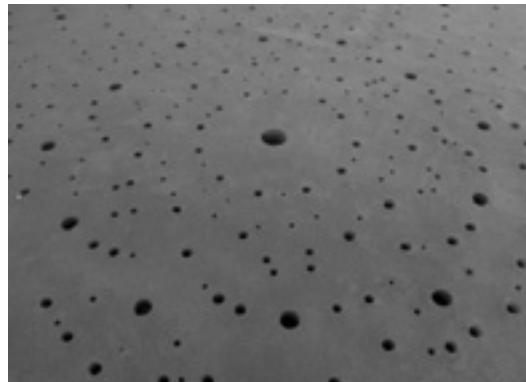
I hope that you enjoy reading this issue of *Crystallography News*.

David Keen

P.S. A puzzle for you to mull over during your Christmas holiday break – who somewhat surprisingly wrote “I do not want to label myself a crystallographer as against a physicist and think indeed that though my research is concerned with crystals it is the physical side of it which attracts me.”



Anna Warren (left) and **Sam Callear** (right) about to make the first Bragg spot in our quartz Laue sand ‘sculpture’.



Close up of the sandy quartz diffraction pattern taken from beach level.

BCA Council 2014

COUNCIL OFFICERS



President (2015)
Prof David Keen
ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, Didcot Oxfordshire, OX11 0QX
Tel: 01235 446556
david.keen@stfc.ac.uk



Vice President (2016)
Dr Richard Cooper
Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford, OX1 3TA
Tel: 07525 687431
richard.cooper@chem.ox.ac.uk



Secretary (2016)
Dr Claire Wilson
School of Chemistry, Glasgow University, Joseph Black Building, University Avenue, Glasgow, G12 8QQ, Scotland.
Claire.wilson.2@glasgow.ac.uk



Treasurer (2017)
Dr Pamela Williams
Astex Pharmaceuticals
436 Cambridge Science Park, Milton Road, Cambridge, CB4 0QA
Tel: 01223 226232
pamela.williams@astx.com

ORDINARY MEMBERS



Prof Simon Parsons (2015)
Room 90, King's Buildings, University of Edinburgh, West Mains Road, Edinburgh, EH9 3JJ
Tel: 0131 650 5804
s.parsons@ed.ac.uk



Dr Andrea Thorn (2016)
MRC Laboratory of Molecular Biology
Francis Crick Avenue
Cambridge Biomedical Campus
Cambridge CB2 0QH
Tel: 01223 267828
andrea.thorn@web.de



Dr Amber L Thompson (2017)
Department of Chemistry, University of Oxford, 12 Mansfield Road, Oxford OX1 3TA
Tel: 01865 285018
amber.thompson@chem.ox.ac.uk

GROUP REPRESENTATIVES



Biological Structures
Dr John McGeehan
Biophysics Laboratories, School of Biological Sciences, University of Portsmouth, Portsmouth, PO1 2DY
Tel: 02392 842042
john.mcgeehan@port.ac.uk



Chemical Crystallography
Dr Pascal Parois
Chemical crystallography, Department of Chemistry, University of Oxford
pascal.parois@chem.ox.ac.uk



Industrial
Dr Elizabeth Shotton
Diamond Light Source
Diamond House, Didcot Oxfordshire, OX11 0DE
Tel: 01235-778797
elizabeth.shotton@diamond.ac.uk



Physical Crystallography
Dr Paul Saines
Department of Chemistry, University of Oxford, South Parks Road, Oxford OX1 3QR
Tel: 01865 272698
paul.saines@chem.ox.ac.uk



Young Crystallographers
Dr Scott McKellar
School of Chemistry
The University of Edinburgh
West Mains Road, Edinburgh, EH9 3JJ
Tel: 0131 650 4804
smckellar@staffmail.ed.ac.uk

CO-OPTED MEMBERS



Bursary Co-ordinator
Dr Alexandra Griffin (2015)
Rigaku Life Science, Unit B6, Chaucer Business Park, Watery Lane, Kemsing, Sevenoaks, Kent TN15 6QY
alex.griffin@rigaku.com



Education & Outreach
Dr Sam Callear (2017)
ISIS Facility, Rutherford Appleton Laboratory, Harwell Oxford, Didcot Oxfordshire, OX11 0QX
Tel. 01235 445162
Sam.Callear@stfc.ac.uk

GROUP CHAIRS



Biological Structures
Prof Vilmos Fulop
School of Life Sciences, University of Warwick, Coventry, CV4 7AL
Tel: 024 7657 2628
vilmos@globin.bio.warwick.ac.uk



Chemical Crystallography
Dr Simon Coles
Chemistry, Faculty of Natural and Environmental Sciences, University of Southampton
Southampton, SO17 1BJ.
Tel: 023 8059 6721
S.J.Coles@soton.ac.uk



Industrial
Dr Cheryl Doherty
Principal Scientist at Pfizer
IPC009
Ramsgate Road, Sandwich, Kent, CT13 9NJ
Tel: 01304 616161
cheryl.doherty@pfizer.com



Physical Crystallography
Dr Matt Tucker
Rutherford Appleton Laboratory, Harwell Oxford, Didcot Oxfordshire OX11 0QX
Tel: 01235 445581
matt.tucker@stfc.ac.uk



Young Crystallographers
Dr Scott McKellar
School of Chemistry
The University of Edinburgh
West Mains Road, Edinburgh, EH9 3JJ
Tel: 0131 650 4804
smckellar@staffmail.ed.ac.uk

EX-OFFICIO MEMBERS



Editor
“Crystallography News”
Prof Carl H Schwalbe
15 St. Augustine Drive, Droitwich, Worcs, WR9 8QR
Tel: 01905 775257
carlschwalbe@hotmail.com



Webmaster
Dr Scott McKellar
School of Chemistry
The University of Edinburgh
West Mains Road, Edinburgh, EH9 3JJ
Tel: 0131 650 4804
smckellar@staffmail.ed.ac.uk

(The dates in parentheses indicate the end of the term of office).

Full committee details on the BCA website www.crystallography.org.uk

From the Editor



THIS issue carries reports about the memorable Congress of the International Union of Crystallography in the International Year of Crystallography. Held in the spacious Palais des congrès de Montreal, the meeting was complemented by and had to compete with the numerous cultural attractions, delicious food and impressive scenery on

offer. A long-lasting heat wave dispelled any preconceptions about Canada being a cold country. Warm sunshine tempted us to take an early morning walk, but in the afternoon the heat impelled us to go to a lecture – any lecture – to enjoy the air conditioning. The inordinately high price of beer at the Palais des congrès meant that, like the European Crystallographic Meeting in Bergen, this was a sober meeting. However, the sobriety did not impair the buzz of scientific creativity.

Before I went to Montreal, I devoted much thought and a column-inch or two to anticipating the culinary delights of poutine (chips with curd cheese and gravy). This delicacy has fortified many a habitant to do hard farm work in the challenging climate of Quebec. Because of a lack of opportunity and/or a lack of courage, I never did try it. However, our picture by **Joshua Hill** shows poutine being consumed with gusto. The sustenance it provided to **Joe Paddison** helped him to give a brilliant presentation. As for our dietary adventures, Joan and I enjoyed a lot of delicious salmon on our post-conference trip around the Gaspé Peninsula. Even a fish soup and a fish salad included lovely meaty chunks of salmon, not scraggy bits of salmon or pieces of unidentifiable generic fish.

The Montreal Congress was attended by almost “everyone who is anyone” in crystallography and covered an amazing variety of topics in its multifarious microsymposia. However, finding the person one wanted to meet in the midst of the throng could be difficult, and all too often one could be torn between two equally interesting simultaneous sessions. These problems will be much less serious at our forthcoming BCA Spring Meeting, which in many ways is the ideal size: big enough to offer topics that will interest every participant but small enough for people to meet and discuss things. As the announcement in this issue shows, the Programme Committee has put together an extremely interesting programme that will appeal to every crystallographer. Features that particularly impress me are the variety of useful workshops on offer and the number of joint sessions which prove the worth of having a society embracing all aspects of crystallography.

Before the calendar year 2014 is finished, the British Biophysical Society will commemorate the close of the International Year of Crystallography with a one-day symposium entitled “Complementary Non-diffraction Techniques in Structural Biology”. It will take place on 11 December from 10.30 to 16.30 at the Brunei Gallery, SOAS, Russell Square, London WC1H 0XG. See page 19 for the meeting of our own BSG in Grenoble from 15-17 December.

Of course, at this time of short days and long nights one does not think only about going out to attend meetings. It can be very pleasant to stay home, seated in front of a nice warm fire

and cuddling one’s laptop. Good reading matter is ready to hand: we now have most of a year’s worth of IUCrJ available on-line. As promised, this journal acquaints us with cutting-edge developments across wide fields of crystallography. Each reader will have a personal set of favourites. Mine include an article by **Louis Farrugia**, whose WinGX software brought structure determination and visualisation conveniently to our laptops, on obtaining accurate H-atom parameters from X-ray diffraction data – something I previously thought was impossible. Those of us who were inspired by the description at a previous meeting of the CheMin X-ray instrument on Mars by the “**Two Davids**” (**Bish** and **Blake**) can find a full account in IUCrJ. This article provides more detail about small but mighty CheMin and also makes clear the amount of careful analysis needed to identify minerals from the data beamed back from Mars. We are also brought up to date with newest developments involving MOFs, under high pressure as well as ambient conditions, and with serial macromolecular crystallography using synchrotron as well as FEL X-ray sources.

Crystallographic history, particularly the remarkable contribution made by the Braggs, has been well illustrated recently in a 40 minute film produced by Diamond Light Source in collaboration with the Royal Institution of Great Britain. A description and some still photos appear at the website <http://www.diamond.ac.uk/Home/News/LatestNews/02-09-14.html>, and the video can be accessed there or at <http://www.richannel.org/the-braggs-legacy>. Good audio material is available, too. As well as **Elsbeth Garman**’s illuminating and heart-warming interview already mentioned by our President, **Georgina Ferry**’s 5 x 15 minute mini-series presents the correspondence of **Dorothy Hodgkin**. The first episode is accessible at <http://www.bbc.co.uk/programmes/b04k9gj1>, and further episodes are accessible from there.

As an American resident of the United Kingdom, I must express my admiration for the civilised way in which the question of Scottish secession was resolved. Of course, the USA had its own issue with secession, which was finally resolved 149 years ago in a far less civilised manner. Still, with the possible exceptions of **Alex Salmond** and the re-invigorated **Gordon Brown**, I didn’t find that the Scottish campaign brought to public attention any larger-than-life figures like **Robert E. Lee** or **Ulysses S. Grant**. Nor were there any tunes as catchy as “Dixie” or “Marching through Georgia”. With secession having met the same fate both times, BCA members can relax and forget about the questions I raised in our September issue. If, decades from now, there is another referendum, I trust that there will be a dusty digital archive where one can consult that article as a PDF, yellowing and curling at the edges but still legible.

This International Year of Crystallography marks a special anniversary for me personally. I have been a practitioner of structure determination by X-ray diffraction for exactly half a century. It’s a sobering thought that this is almost half the time that the technique of X-ray diffraction has existed, but it pales into insignificance compared to the length of service that **Stephen Wallwork** has enjoyed. I am delighted to publish in this issue his account of his early days as a crystallographer.

Carl Schwalbe



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The BCA values its close ties with commercial companies involved with crystallography. To enhance these contacts, the BCA offers Corporate Membership. Corporate Membership is available on an annual basis and includes the following benefits:

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- Influence on the development of crystallography and the BCA

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Puzzle ‘Poets’ Corner



THE passing of an old year inevitably brings a feeling of sadness, which we try to counteract with light-hearted entertainment such as parties and pantomimes.

With a gadget we call F.E.L.,
Though it blasts every crystal to hell,
Just a minuscule jet
Gives a full data set
And a paper in *Nature* as well.

A clever young fellow named Bragg
Measured X-ray reflections from slag.
Reflections are bright
If the phases are right
But not if they lead or they lag.

Editor's note: Lawrence Bragg actually determined the structures of many silicates [W. L. Bragg, "Atomic Arrangement in the Silicates" in *Transactions of the Faraday Society*, **25** (1929). 291–314], but none of them rhyme with Bragg. Therefore, I had to use a generic term.

An eager young German named Max
On the nature of X-rays sought facts.
With Friedrich and Knipping,
By turning and tipping,
He showed that a crystal diffracts.

The inveterate puzzle-solvers among you will find one at the end of our President's article.

Answer to June Puzzle

From page 34 of the June issue:

A CENTURY OF CRYSTALLOGRAPHY

1. Von Laue, Pauling, Hodgkin, Lipscomb, Klug, Yonath.
2. Nobel Prize.
3. Ada.
4. $1914 + 1954 + 1964 + 1976 + 1982 + 2009 + 100 = 11899 = 11$ August 1999.
5. Total eclipse of the sun.
6. Glasgow, IUCrXVIII.

BCA Annual Spring Meeting

University of York, 30 March – 2 April, 2015



From the BCA 2015 Programme Committee

WE invite you to the University of York in the springtime of 2015 for a diverse and exciting meeting featuring talks, posters, workshops and a commercial exhibition. You are invited to submit an abstract for a talk in any of the sixteen topical micro-symposia. In addition we offer a 'General and Hot topics' option, and depending on demand we may run extra micro-symposia.

The 2015 BCA Named Lecturers are:-

Dorothy Hodgkin Lecture:

Prof. Sir Tom Blundell FRS.

"Dorothy Hodgkin, Structural Biology and Drug Discovery"

Lonsdale Lecture:

Prof. Simon Parsons.

"High Pressure and the Molecular Crystalline State"

The Plenary speakers are:-

BSG: **Prof. Gideon Davies FRS,** University of York

CCG: **Dr. Colin Groom,** CCDC

IG: **Dr. Peter Chupas,** APS, Chicago

PCG: **Prof. Anthony Cheetham FRS,** University of Cambridge

The biological structures component of the meeting spans all six parallel sessions. The layout of the York Exhibition Centre also allows us to run workshops simultaneously with sessions, allowing plenty of further choice for delegates.

This year we have scheduled two events to capture the recent surge in outreach and education activities by the BCA. There will be an educational lecture during the Young Crystallographers' Satellite Meeting in the form of a double

act by Prof. **Mike Glazer** and Prof. **Bill Clegg** on the use of International Tables for Crystallography. Secondly there will be a session within the main meeting dedicated to the subject of teaching crystallography.

For the first time at a BCA, workshops will run simultaneously with all sessions. There will be a dedicated room for these hands-on workshops which will be accessible at all times. The scheduled workshops provide many exciting opportunities to gain first-hand experience with a wide range of crystallographic software:

- Diffractometer software: Agilent, Bruker, Rigaku and STOE
- Small Molecule software: CRYSTALS, Olex2, XPAC and the CCDC
- Biological Molecule software: CCP4.mg, DIALS; PDBe Roadshow
- Physical Chemistry: Symmetry Modes

Whether you are a student starting out in crystallography, or somebody who uses these tools as part of your everyday working life, you are sure to benefit from these practical and informal sessions. We will have access to the workshop rooms throughout the conference and hope that learning doesn't stop when the presentations finish!

Meeting website:

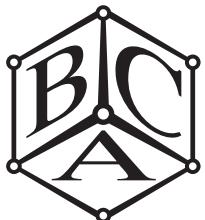
<http://york2015.crystallography.org.uk/>



Registration and Abstract Submission deadlines

The registration is now open.

The deadline for oral abstract submissions, including submission for the YCG Satellite Meeting, is **Monday 12 January, 2015**. The final deadline for poster abstracts is **Monday 2 March, 2015**.



Scientific Programme

Monday 30 March 2015 pm
and **Tuesday 31 March am**

Young Crystallographers Group Satellite Meeting



Confirmed Plenary speakers:

Prof. Susan Lea
Prof. Bill David

Space groups teaching sessions: Prof. Bill Clegg and Prof. Mike Glazer

Main Meeting Tuesday March 31, 2015

12 noon to 12:50pm

Dorothy Hodgkin Lecture:
Prof. Sir Tom Blundell FRS.

"Dorothy Hodgkin, Structural Biology and Drug Discovery"

1:30pm to 2:20pm

CCG Plenary:

Colin Groom, CCDC.
"Fifty years of sharing crystal structures".
Chair: Simon Coles

2:30pm to 4:00pm

BSG: Drug design

Chair: Dave Brown (Kent)

CCG: Data Avalanche

Chair: Mark Warren (Diamond), Co-chair: László Fábián (University of East Anglia)

Keynote: Peter Galek (CCDC)

With the dramatic decrease in read out times of detectors the time to obtain a dataset has also dramatically reduced. An entire dataset can now be collected in a matter of milliseconds at synchrotrons and tens of minutes in-house. With this, the crystallographer has been bombarded with shed loads of data! How will we cope? Well, the "Data Avalanche" session will bring together experienced speakers who have come up with strategies to organise and compare all their processed data, and ways in which the vast number of resulting structures can be evaluated and summed up in manageable tables and graphs.

PCG: Beyond the Elastic Line – Resonant and Inelastic Diffraction

Chair: Mark Senn (University of Oxford)

Keynote: Steven Collins (Diamond) "Resonant X-ray Diffraction and the elusive sign of the DM interaction in weak ferromagnets"

This is an interdisciplinary session designed to bring crystallographers together with researchers who come from a background in resonant and inelastic scattering. The aim of the session is to explore the possibilities in crystallography beyond "conventional" charge scattering, and speakers with a background in spectroscopy or an element of spectroscopic measurements in their work are strongly encouraged to apply.

Workshops: Diffractometer software: Agilent, Bruker

4:30pm to 6:00pm

BSG: Data acquisition

Chair: Elspeth Garman (Oxford).

Keynote: Gwyndaf Evans (Diamond) "Exploring the limits of synchrotron radiation in macromolecular crystallography"

CCG: Automation

Chair: Claire Wilson (Glasgow), Co-chair: Pascal Parois (University of Oxford).

Keynote: Graeme Winter (Diamond)

Developments in areas such as detectors, sources and computing provide powerful drivers for automation in chemical crystallography. Automation also offers exciting opportunities to carry out new systematic scientific studies. This session could include work relating to hardware and/or software to handle higher throughput of structures and results of studies arising from such developments.

PCG: Challenges and Technical Advances in Powder Diffraction

Chair: Paul Saines (University of Oxford).

Keynote: Pascal Manuel (ISIS) "Extreme Conditions and Magnetic Neutron Diffraction: how far can we push it?"

Powder diffraction plays a crucial role in the characterisation of functional materials including studies in-situ and at extreme conditions; especially in the many cases where single crystals are unavailable. This session will examine recent developments

in techniques and instrumentation alongside cutting edge results in this important field.

Workshops: Diffractometer software: Rigaku and STOE

6:10pm to 7:00pm

BSG Plenary:

Prof. Gideon Davies FRS, University of York. "Probing the reaction pathways of enzymes through crystallography"
Chair: Prof. Eleanor J Dodson FRS

7:00pm

Buffet dinner, Exhibition and Posters.



Wednesday April 1, 2015

9:00am to 9:50am

PCG Plenary: Prof. Anthony Cheetham FRS (University of Cambridge) "Phase Transitions in Metal-Organic Frameworks"
Chair: Matt Tucker (ISIS/Diamond).

10:15am to 12:15pm

Student Prize Lectures

Workshops: BSG (PDBe Roadshow); PCG (Symmetry modes)

1:30pm to 3:00pm

BSG and CCG Joint micro-symposium

Chair: Ehmke Pohl (Durham University), *Co-chair:* Jason Cole (CCDC).

Keynote: Prof. Martin Noble (University of Newcastle)

This session is focussed on the interface between chemical and macromolecular crystallography where structural information from the entire range of crystallography is used to analyse, understand and optimise small-molecular to protein interaction. We welcome presentations describing novel methods and experimental techniques, as well as current examples of important protein-ligand systems.

IG: Catalysis

PCG: Structural Insights into Ferroic Materials

Chair: Phil Lightfoot (University of St Andrews).

Keynote: Pam Thomas (University of Warwick) "Structures and Properties of Lead-Free Piezoelectrics – Domains, Disorder and Disagreements."

Materials that undergo phase transitions to ferroelectric, ferroelastic or (ferro)magnetically ordered states are technologically vital. This session will focus on the nature of these phase transitions, the symmetry breaking that occurs and the possibility of coupling these ferroic orders.

Workshops: Small Molecule software: CRYSTALS & Olex2

3:30pm to 5:00pm

BSG: Data Mining – wealth & pitfalls

Chair: Kevin Cowtan (York).

Keynote: Dr. Robbie Joosten (Netherlands Cancer Institute).

CCG & PCG: Complementary Calculations

Chair: John Claridge (University of Liverpool), *Co-chair:* Simon Parsons (University of Edinburgh)

Keynote: Keith Refson (STFC Rutherford Appleton Laboratory)

The use of computational methods has made great strides, both in structure determination, prediction of new structure types and their response to stimuli, providing insight and guidance to experimental studies. We welcome presentations on computational methods used to complement traditional crystallographic techniques to give a deeper understanding of crystal chemistry and physics.

Education Session: *Chair:* Mike Glazer

Keynote: Juliette Pradon (CCDC) "Crystallographic education and research in the developing world: Experiences in the Democratic Republic of the Congo"

Workshops: Small Molecule software XPAC and CCDC

5:10pm to 6:00pm

Lonsdale Lecture:

Prof. Simon Parsons

"High Pressure and the Molecular Crystalline State"

6:00pm to 7:00pm

BCA AGM

7:30pm for 8:00pm

BCA Conference dinner.



Thursday April 2, 2015

9:00am to 9:50am

IG Plenary: Dr. Peter Chupas, APS, Chicago. "Hard X-ray Studies of Materials for Energy Storage and Conversion"

10:15am to 11:45am

BSG: Simultaneous use of EM and MX data

Chair: Garib Murshudov (LMB, Cambridge).

Keynote: Alan Brown (LMB, Cambridge) "Cryo-EM at near atomic resolution - recent developments in model building, refinement and validation"

CCG: Problem Data

Chair: Stephen Moggach (University of Edinburgh), *Co-chair:* Jamie Gould (University of Liverpool).

Keynote: Andrew Goodwin (University of Oxford)

Recent advances in crystallographic software and hardware have resulted in significant advances within many areas of crystallographic research. These include time resolved studies, experiments involving different sample environments and the extraction of detailed information from between the Bragg reflections. We welcome presentations on methods which involve extracting crystallographic information from such sample environments on what are (or once were) referred to as 'problem data'.

IG - PCG Joint Session: Amorphous Materials, Nanomaterials and Liquids (Part 1)

Chairs: Christoph Salzmann (University College London) and Spoorthi Dharmayat (LGC Group).

Keynote: Dr. Sam Callear (ISIS)

Lacking long-range order, liquids, nanomaterials and amorphous materials are notoriously difficult to characterise structurally. From a technological and scientific point of view they are, however, immensely important classes of materials. This double session will highlight some of the recent advances in this area ranging from structural characterisations to the applications of these materials.

Workshops: Biological molecules CCP4mg

12noon to 1:30pm

BSG: Low-resolution refinement

Chair: Keith Wilson (York).

Keynote: Steven Johnson (Oxford University) "Through the Distorted Looking Glass: tales of low resolution refinement."

CCG: Would you publish this?

Chair: Bill Clegg (University of Newcastle), *Co-chair:* Gary Nichol (University of Edinburgh).

Keynote: Larry Falvello (University of Zaragoza)

This session will have an unusual format. After an opening talk by Prof. Larry Falvello from the points of view of a crystallographer, author, and editor, anyone present can briefly describe one or more structural results that raise the session title question for

the audience to discuss, with the aim of constructive rather than negative criticism. We particularly encourage submissions from Young Crystallographers. Problems might include charge imbalance or other chemical issues, low resolution or data completeness, tricky disorder, highly restrained models, residual electron density and other artefacts, etc. A formal abstract is not required, but please contact the session organisers in advance of the meeting (as soon as possible!) if you wish to contribute; we will request 1–3 slides for concatenation into a single session presentation.

IG - PCG Joint Session: Amorphous Materials, Nanomaterials and Liquids (Part 2)

Chairs: Christoph Salzmann (University College London) and Spoorthi Dharmayat (LGC Group).

Keynote: tbc

Part 2 continues the presentations on this big theme made in Part 1.

Workshop: Biological molecules: DIALS, POINTLESS, AIMLESS and cTRUNCATE

John R Helliwell

(Chair of BCA 2015, john.helliwell@manchester.ac.uk) and

Richard Cooper

BCA Vice President, richard.cooper@chem.ox.ac.uk)



Summary of the Workshops timings (tentative):-

Tue pm 1	How to get the most out of CrysaliisPro (Agilent) APEX2 Software Suite – The must-have solution for crystallography (Bruker)
Tue pm 2	Rigaku Software for Data Collection and Processing (Rigaku)
	STOE data collection/reduction software (STOE)
Wed am 1	Symmetry Modes (Branton Campbell)
Wed am 2	PDBe Roadshow
Wed pm 1	CRYSTALS (Pascal Parois, Richard Cooper)
	Olex2 (Oleg Dolomanov, Horst Puschmann)
Wed pm 2	XPac (Thomas Gelbrich)
	CCDC (Pete Wood)
Thu am 1	CCP4.mg (Stuart McNicholas, KSW)
Thu am 2	DIALS (David Waterman)
	Data Quality: POINTLESS, AIMLESS and cTRUNCATE

The BCA 2015 Programme and Organising Committee is:-

John R Helliwell (Chair)

Eleanor Dodson FRS (BSG & Workshops)

Keith Wilson (BSG)

Mike Probert (CCG)

Pete Wood (CCG)

Spoorthi Dharmayat (IG)

Judith Shackleton (IG)

Emma McCabe (PCG)

Paul Saines (PCG)

Horst Puschmann (Computing and software & Workshops)

Scott McKellar (YCG)

Lucy Saunders (YCG)

Claire Wilson (BCA Secretary)

Richard Cooper (BCA Vice President)

David Keen (BCA President)

The IUCr Congress in Montreal

THE 23rd Congress of the International Union of Crystallography opened spectacularly on August 5. We had the usual warm and eloquent welcoming speeches, but interspersed among them were acrobatic displays by members of Montreal's Cirque Éloize (*Éloize* means "heat lightning" in Acadian French). As if daredevil ascents into the third dimension high above the 2-dimensional podium did not make us gasp enough, **Ted Janssen** of the University of Nijmegen, The Netherlands, took us into superspace crystallography in his Ewald Lecture. With his colleague **Aloysio Janner** he shared the 10th Ewald Prize awarded by the IUCr. The next day a very full programme of talks and posters began. Inevitably I can only highlight a few sessions. I am grateful to **Matt Dunstan** for supplying information on behalf of the Physical Crystallography Group, to **Richard Cooper** for an account of MS96 and to our bursary recipients for contributing their reports.

I chose to start with MS05, "The Crystallography of HIV/AIDS". In a presentation about substrate envelope based drug design against HIV and hepatitis C proteases **Celia Schiffer** made some important points. Since the residues in the immediate vicinity of the substrate are likely to be essential for function, an inhibitor which binds there should retain its effectiveness. Any mutations of the relevant amino acids which prevent inhibitor binding should also abolish function and therefore be clinically irrelevant. Groups protruding from the active site can provide additional binding targets that enhance inhibitor affinity. However, this approach is risky because mutation of those amino acids can expel the inhibitor without abolishing function. **Peter Kwong** told us about long-sought progress in defining the structure of the HIV-1 Env spike, which is the target for most antibodies with broad HIV-1 neutralising ability. It consists of three gp120 and three gp41 subunits. Low-resolution studies with electron microscopy, NMR and X-ray crystallography had demonstrated conformational changes upon association of monomers to form trimers, receptor binding and membrane fusion. X-ray diffraction data to 3.5 Å have recently been obtained on the entire prefusion spike. Binding of antibody 35O22 fixes the orientation of proteins that otherwise would move. **Karen Siu** presented the crystal structure of another of our defences against retroviruses in general and HIV-1 in particular. The APOBEC3 family of cytosine deaminases binds to single-stranded DNA, stalling reverse transcriptase and deaminating cytosine to uracil. However, the viral infectivity factor (Vif) of HIV-1 targets APOBEC3s for proteasomal degradation. Structure-guided mutagenesis has revealed that negatively charged as well as hydrophobic residues facilitate Vif binding, thus suggesting possible targets for development of inhibitors of such binding. **Ron Diskin** turned to the rational design of antibodies. All too often the antibody response against the HIV-1 spike is not very effective. Starting with NIH45-46, one of the most potent anti CD4 binding site antibodies, a region in the inner domain of gp120 was identified as important for its binding. Mutating glycine 54 of this antibody to tryptophan generated additional

binding to a hydrophobic pocket on the surface of gp120, the resulting antibody being the most potent and broadly neutralising anti HIV antibody known. Development of this antibody provides hope for passive immunisation.

The next day featured a microsymposium (MS30) entitled "Data to Knowledge: How to Get Meaning from Your Result", which addressed a particular interest of mine. We can take pride in the ever-growing torrent of structure determinations, on macromolecules as well as small molecules, that our community is producing; but how can we make best use of all this information? Starting at the most "macro" end, **Jack Johnson** described VIPERdb, the Virus Structural Database, and used it to explain virus maturation. The database has useful tools such as Gallery Maker, a GUI for intra-family comparison. Maturation can be analysed in terms of protein-protein interaction and protein dynamics. Next, **Torsten Schwede** discussed the modelling of protein structures. There is a "protein structure gap" between structures in the PDB *versus* sequences in SwissProt *versus* DNA sequences. From the "physics" perspective the native conformation is a global free energy minimum. From the "biology" perspective homologous proteins evolved from a common ancestor. For homology modelling it is important to select an appropriate template. Except in restricted applications, algorithms do better than "gurus". **Matthew Zimmerman** introduced LabDB. This database can integrate data from different makes of equipment and keeps track of every chemical a protein has encountered. Such information may enable the attribution of otherwise mysterious electron density peaks. **Helen Berman** emphasised that the Structural Biology Knowledge Base, although it was designed for the Protein Structure Initiative, will live on after it and will provide an integrated resource for all biologists. It is searchable by sequence and structure, and also by function or disease. Topic driven hubs, e.g. "membrane proteins", collect services for users. **Robert Nicholls** told us about conformation-independent structural comparison with PROSMART, which is available through CCP4. Examples include comparison of homologues to cluster their spatially-conserved regions. Examination of ligand-induced conformational states aids the identification of hinge residues. Finally, **Colin Groom** provided the bridge between small-molecule and macromolecular data. Analysis of alternative conformations of moieties occurring frequently in the Cambridge Structural Database (CSD) shows that frequency of occurrence gives a good inverse correlation with energy. The intersection of CSD structures and ligands in the Protein Data Bank (PDB) is about 16%, facilitating comparison. Occasionally a small molecule is genuinely strained when bound to a protein (that is about to break it). However, Colin drew the memorable conclusion that, in general, protein crystallographers rather than proteins are responsible for strained small molecules.

The keynote lecture (KN29) by **Mark Spackman** on "Rationalising Molecular Crystal Structures using Hirshfeld Surfaces" joined up well with a subsequent session on education (MS84). Hirshfeld surface analysis as pioneered by

the Spackman Group has become a standard technique for visualising shape complementarity. It has now been extended to make explicit the previously useful but somewhat vague concept of electrostatic complementarity, by mapping the electrostatic molecular potential onto the Hirshfeld surface. Provided that a realistic estimate of the dispersion contributions can be made, information becomes available about the relative strengths of electrostatic interactions, and an “energy framework” can be used in discussions of packing motifs. The ensuing microsymposium, “Crystallography Education and Training in the 21st Century: New Pedagogies, New Paradigms...” began with a talk by **Horst Puschmann** on “Structure Determination in a Changing World”. If we are to accommodate increases in population and energy use, we need new materials and processes, the development of which requires structural information from crystallography. This growing need for structures is being met, not just by professionals, but more and more often by untrained people. Therefore we need careful validation, but software must also help to forestall errors in the first place. For instance, 97% of small-molecule structures are refined with SHELX, and SHELX does a good job of treating a disordered aliphatic OH group – if the user knows how to set up the necessary PART 1, PART 2 and PART 0 instructions in the correct order. A lot of teaching, and continuing care and attention by the user, can be avoided if this work is done automatically and checked visually. Crystallographic education should start with how to get a good quality structure and how to spot errors. **Erin Wasserman** showed that, for talented students, scientific research can begin already in high school. In upstate New York about 40 15- and 16-year olds participate in joint research with established scientists, do job-shadowing and attend summer camps. In extracurricular activities spanning the rest of their high school careers they begin with a literature survey and finish by presenting their research results after training by an actor. **Alexander Nazarenko** returned the discussion to college level but with respect to students who will not become specialist crystallographers. Nevertheless, as general chemists, forensic scientists or art conservators they will need to apply crystallography as an indispensable analytical tool to identify unknown (poly)crystalline samples. The lecture course is structured appropriately, and as much experimental work as possible is shown. Under the title “Educational Outreach and User Training at the wwPDB” **Matthew Conroy** and **Christine Zardecki** described the online resources collected at “PDB101” to promote a structural view of biology. Along with the ever-popular “Molecule of the Month” there are resources for making paper models and a PC game on amino acids. The PDB itself has been made easier to access (for instance, someone interested in the ribosome does not have to look up every component). The wwPDB Foundation supports student travel. The final two talks dealt with the vital but sometimes contentious business of fitting ligands to proteins. Structure-based drug design gives hope for re-invigorating the discovery of new drugs but will do nothing but mislead if the ligands are incorrectly located. **Ethan Merritt** told us “When good ligands go bad” and warned us that up to a third of the ligands in the PDB are wrong in some way: bent out of shape, in the wrong place, or should not be there at all. After a lot of effort, tools for validating protein structures are mature and widely used for validation. Recently the PDB also began validating ligand geometry. The results can come as a nasty surprise to crystallographers. Tools such as cprodrg, available through CCP4, and Grade, provided by Global Phasing Ltd., help with the generation of suitable ligand restraints; but even these can be fallible. **Bernhard Rupp** concluded with “Ligands of

fancy”. He began with two important definitions. A *paradigm* is a universally valid set of practices in a scientific discipline. *Epistemology* constitutes the rules of acquiring knowledge in the process of inductive inquiry. Science generates knowledge in two ways. The Baconian method is discovery based; experimental results add to knowledge in a way that is disorganised but safe. Starting in the 18th century, the hypothesis based method was used. The necessity then arose of dealing with negative results that contradicted the hypothesis: they could be wrong or they could spark a scientific revolution; but the temptation is simply to ignore them. The binding site of a protein wants to bind something, but this could be buffer components which, through wishful thinking, could be misinterpreted as a desired ligand. The Bayesian approach provides a survival guide: likelihood (e.g. of a model) is related to the product of the quality of evidence (e.g. the fit to electron density) X prior probability (e.g. the rules of stereochemistry).

Carl Schwalbe

MS-96: New computational approaches to structure solution and refinement

Number of attendees: variable between 160 and 250

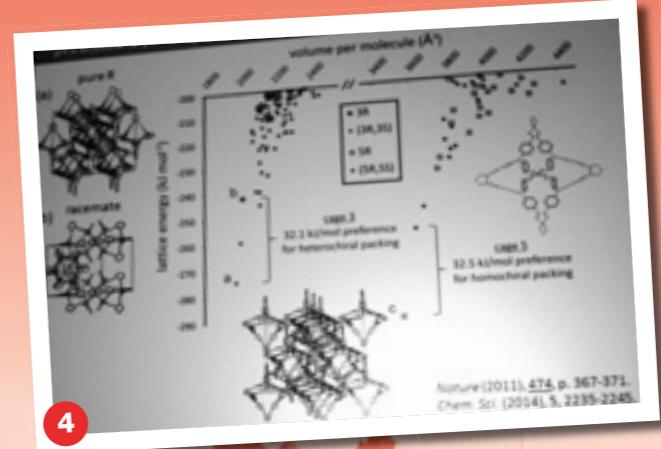
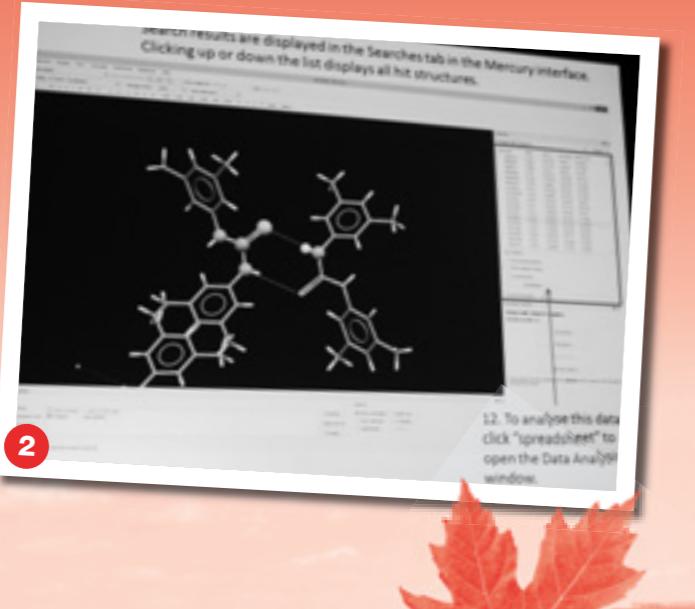
Structure determination still remains the key step in most crystallographic analyses. This microsymposium gathered contributions dealing with this problem from several perspectives and on various types of materials. **Julien Jorda** presented a crowdsourcing approach to phasing macromolecular structures using the pattern recognition capacities of humans. The contributions of **Matt Tucker** and **Pavol Juhas** focused on the determination of local structure and structure of nanoparticles using a combination of techniques, where the dominant analysis of pair-distribution function is assisted with other techniques like small angle scattering, EXAFS or NMR.

Briony Yorke described the application of Hadamard matrix transformations to collecting time-resolved data of photocaged macromolecules. Finally, **Ton Spek** and **George Sheldrick** gave an account of their latest work in the field of structure determination of small-molecule structures. Ton Spek presented the integration of the SQUEEZE method with the newest version of the refinement program SHELX2014, while George Sheldrick presented the basic principles of the program SHELXT, which should be used, in the author’s own words, as the replacement of the very successful structure solution program SHELXS.

The microsymposium demonstrated that the question “where are the atoms?” is still of utmost importance and that active research into a wide variety of methods is going on in this field. The large audience present at this microsymposium is the proof of the wide interest in this question among the delegates of the IUCr 23 Congress.

Richard Cooper
University of Oxford

Reports continued on page 14.



PICTURE CAPTIONS:

- 1 Pete Wood
2 Pete Wood's slide
3 Ewald lecturer Ted Janssen
4 Graeme Day's slide
5 Graeme Day
6 Colin Groom
- 7 IUCr/IYCr booth
8 Welcome from local organisers
9 Basilica
10 Participants in the exhibition area
11 Olympic Stadium and Montreal Tower
12 OpenLabs

This year saw my first time attending the International Union of Crystallography (IUCr) Congress and General Assembly, which was hosted by Montreal for its 23rd edition. The meeting started even before I had boarded my flight, running into **David Keen** and the Goodwin group at the check-in at Heathrow, and I got a small taste of the camaraderie that comes from making new friends and catching up with old ones in the crystallography community (a feeling that would last through the entire conference).

IUCr 2014 was certainly a daunting conference on paper – 7 full days featuring over 750 oral presentations and 1500 poster presentations – one of the biggest conferences I have ever been to. At the same time, it was a fantastic opportunity to hear about crystallography from a diverse set of vantage points: chemical, biological, mathematical and even astrophysical, and to see how this central scientific principle unites such a disparate group of researchers.

It is hard to do justice to the high quality of innovative and intriguing science that was presented over the week, but I will do my best to recount some personal highlights. **John Evans** showed us the vast amount of information that can be derived from powder diffraction data; **Branton Campbell** gave an excellent overview of the use of symmetry mode analysis to analyse lower symmetry structures in terms of a higher symmetry structure's distortion modes; **David Bish** recounted his journey building the CheMin instrument on the Curiosity Rover that resulted in the first x-ray powder diffraction measurements on Mars; and **Ray Withers** gave us (in his usual entertaining style) a look into the world of modulated structures, and how sometimes you just have to get your hands dirty and diagonalise a 9 x 9 matrix yourself. There were also a large number of talks reflecting on newer ideas in the crystallography community, including quasicrystals and disordered materials, pushing the boundaries of even the very definition of crystals and order.

It wasn't all work and no play though, and in the evenings we got a chance to explore the vibrant nightlife of Montreal, including its lively Latin Quarter and Harbour districts. I also finally capitulated and tried the local delicacy of poutine, essentially a dish comprising of French fries, gravy and cheese curds, which tasted pretty much as good as it sounds (thankfully I waited until after I had given my talk to try it!).

In the end, the conference was a very rewarding experience, especially when reflecting on the friends I have made in the crystallography community from all over the world, and the truly excellent science I was exposed to. As such, I would like to thank the IUCr Congress for the award of a travel bursary to attend the conference, as well as funding from the Cambridge Trusts and Trinity College, without which I would not have been able to attend.

Matt Dunstan
University of Cambridge

The IUCr 2014 was a unique experience for the delegates. Scientific excellence combined with the excitement of the celebration of the International Year of Crystallography (IYCr2014) made this conference to be remembered. Before the opening ceremony of the conference, the workshop on

XFEL was a valuable introduction to the developments in X-ray crystallography that were extensively presented and discussed during the meeting.

As 2014 has been declared the International Year of Crystallography by the United Nations to celebrate 100 years since the Nobel Prize to **Max von Laue**, there were dedicated micro-symposia talks at the IUCr2014. During 'The Beginnings of Biological Crystallography' session, co-chaired by **Eleanor Dodson** and **Gil Privé**, **Phil Evans**, **Helen Berman**, **Michael Rossmann** and others gave fantastic talks on the history of macromolecular crystallography through their own experiences. The take-home message was that during past century, the impact of X-ray crystallography has been tremendous in biology and the new advances and methodology will keep the crystallographers busy in the future.

The development of advanced X-ray sources was extensively discussed in this conference. The hard and intense XFELs allow diffraction measurements of nanocrystals. The most interesting feature of this X-ray source is that the ultra-short pulse duration makes possible data collection from tiny crystals despite radiation damage. Serial crystallography using synchrotron radiation is also promising for small protein Crystals, and an example was given by **Lars Redecke** in the meeting. The developments in X-ray sources have pushed for new methods and software development to improve the data collection, processing and interpretation. **Gwyndaf Evans** presented a method on how to collect and analyse diffraction data from multiple crystals. **Wayne Hendrickson** gave a memorable talk on how to native-SAD phase multiple crystals. **Pavel Afonine** from PHENIX gave an interesting solution to the problem of weak and ambiguous macromolecular maps by producing a new Featured Enhanced Map (FEM). **Harry Powell** gave an informative presentation on how to do cell refinement and data integration on crystals with multiple lattices. Finally, a great interactive talk was given by **Zbigniew Dauter** on important information on structural flexibility when collecting data at ultra-high resolution.

I was grateful for the opportunity to present a poster about my work entitled 'Structural studies of anti-IgE Fab fragments' and honored to receive the Bernhard Rupp Prize for macromolecular crystallography.

Overall, the IUCr2014 was a most enjoyable event. Speakers and poster presenters from around the world covered a vast range of topics and made this conference a great learning experience. To that end, I would like to acknowledge the BCA and King's College London for their financial support to enable me to attend this special meeting.

Alkistis Mitropoulou
King's College London

August 2014 saw the 23rd Congress and General Assembly of the International Union of Crystallography in Montreal, Canada. The Palais des Congrès provided the perfect location for this special congress in the International Year of Crystallography. This was marked by a public week-long poster exhibition, as well as a screening of an interesting play about the life of **Dorothy Hodgkin** called 'Hidden Glory: Dorothy Hodgkin in her own words'.

The 8 day conference provided sessions on a whole range of topics connected to crystallography, from structure solution techniques to applications to specific problems via complementary approaches, which ensured that there was something to suit everyone's tastes.

My research currently focuses on the prediction of crystallisation propensity of small organic molecules with a view to improving structure solution of these materials, and so a particularly interesting session for me was entitled "Extending the Power of Powder Diffraction for Structure Solution". The session began with a fascinating talk by **Christopher Wolverton**, who proposed that powder diffraction solution techniques could be combined with computational structure prediction methods to improve the overall structure solution process, a great way of taking the best parts of two established methods to solve a problem. **Martin Schmidt**'s talk describing FIDEL, a new method for SDPD of nanocrystalline organic compounds, was equally interesting, as it described a way of fitting with deviating lattice parameters to get the best possible fit to a powder pattern for cases where the lattice parameters are incorrect, and could also be used for low quality diffraction patterns. Finally, **Cory Widdifield** highlighted the value of combining NMR and crystal structure predictions to carry out powder crystallography, which was interesting to see a new method of approaching a structure solution problem.

The other session of most interest to me was "New Approaches to Crystal Structure Prediction". **Sally Price**'s explanation of how to interpret the computed crystal energy landscape of a pharmaceutical molecule to find thermodynamically feasible crystal structures gave a great introduction to the field and the way that the energies are calculated for each polymorph, as well as the current limitations of the method. **Marcus Neumann** then went on to describe a fully automated crystal structure prediction pipeline, which showed how far this field has progressed in recent times. These talks all supported the excellent keynote lecture by **Graeme Day**, which provided a more general overview of the history of crystal structure prediction and the ways in which it is currently being used to predict cocrystallisation of enantiomers and of cage molecules.

The location of the conference allowed for some amazing sightseeing visits during any downtime, with particular highlights being the climb to the top of Mont-Royal, from where there was a wonderful view over the downtown area, and night-time walks along the quay area to the old town and Vieux-Port district. The social events within the conference, such as the buffet dinner on the opening night and the conference dinner, were also welcome networking opportunities as well as being a fun way to relax in the evenings. Overall the conference was

an enjoyable and interesting experience, and the opportunity to present a poster was fruitful as it allowed me to talk to people who were interested in my research. I would like to thank the BCA for awarding me an ABBF bursary, giving me the financial support to make the trip possible.

Jerome Wicker
University of Oxford

It's a good thing that the IUCr Congress comes but every three years as – with over 200 hours of micro-symposia (not to mention keynotes, plenaries, workshops, and satellites!) – it is exhausting: of course in a good way! The 23rd IUCr was held in Montreal, a city with at least two must-see attractions for the structural scientist: **Buckminster Fuller**'s geodesic dome – visible in the distance from the waterside near the conference venue; and 20,000 pink balls in The Village – a fantastic cross-over with Montreal Pride!

This being my first IUCr I was struck by the size and diversity of the meeting. As well as seeing many fantastic talks, a few of which I will mention below, the software sessions given by **Branton Campbell** on ISODISTORT and by **Arkadiy Simonov** on the diffuse scattering interpretation program Yell were both exciting and useful.

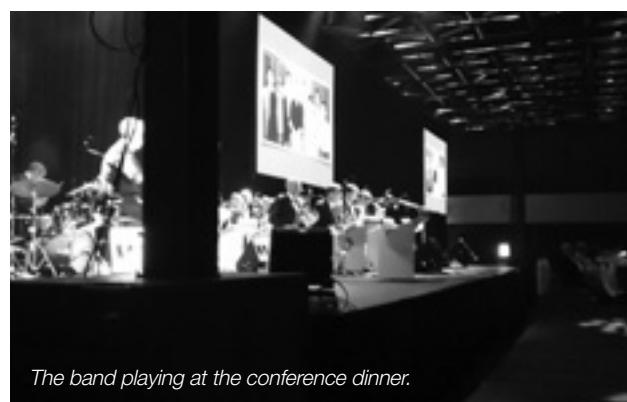
The importance of understanding local structure was a common theme in much of the physical crystallography whether for fundamental or practical interest. In the field of energy materials **Phoebe Allan**, among others, spoke eloquently on antimony anodes for Na-ion batteries and demonstrated the utility of PDF techniques for some extremely complicated systems. In another session, **Karena Chapman** gave a wide-ranging talk on developing in-situ studies of energy storage and conversion materials at the Argonne National Laboratory. Elsewhere, **Marek Paściak** spoke about modelling the diffuse scattering of the important relaxor and incipient ferroelectrics barium titanate and strontium titanate, respectively.

It was a great pleasure to hear the inimitable **Ray Withers** talk. Among the systems he spoke about in his keynote on hidden long range order in nominally 'disordered systems' were NaCl-type magnesium doped rare-earth sulfides. The signature of the 6-body correlations of one particular member of this family manifested not as 'diffuse' scattering but as sharp, continuous 3D shapes in reciprocal space – encoding both long- and short-range order in these non-Bragg features.

Alexander Shtukenberg gave an overview of some other neglected sharp 3D objects – twisted crystals. These crystals forego long-range translational order, twisting and bending as they grow. While most crystallographers would avoid such materials, Shtukenberg showed the great diversity of distortions possible as well as the beauty of the resulting crystals.

Talks were not without humour – even if sometimes lost on the international audience – perhaps most notably **Phil Lightfoot**'s double-act with **Eric Morecambe** explaining mode analysis of some ferroic Perovskites.

A trip to Montreal would not be complete without a serving of poutine - though perhaps not the best food to calm your



The band playing at the conference dinner.

nerves before giving a talk. I am very grateful to the BCA for their support in the form of an Arnold Beevers Bursary and to the chairs of MS83 for giving me the opportunity to speak as a PhD student. I look forward to the 24th IUCr in Hyderabad!

Joshua Hill
University of Oxford

The 23rd Congress and General Assembly of the International Union of Crystallography was held this year in the beautiful Canadian city of Montreal. The venue was the striking Palais des Congrès, situated in the heart of Downtown Montreal adjacent to the vibrant Old Town area of the city. From my arrival on the 4th of August for what promised to be 8 days of stimulating and interesting keynotes, microsymposia and plenaries, this conference did not disappoint.

The conference provided something for everybody, containing talks spanning a wide variety of areas including small molecule, protein and theoretical crystallography. Herein I have highlighted two sessions which were of particular interest to me throughout the conference.

Since my DPhil studies have focused on the application of macromolecular structure solution techniques to small molecule crystallography, the first of my highlighted sessions was "Improving Your Crystallography: Best Practices and New Methods", which included two of my favourite talks of the meeting. The session kicked off with an interesting talk given by **Gwyndaf Evans** explaining how data from multiple crystals can be used in conjunction with the new program BLEND to solve difficult structures. Due to the popularity of the session, it was then relocated to a larger room for a second fascinating talk by **Wayne Hendrickson**, highlighting the merits of using multicrystal SAD phasing over conventional molecular replacement techniques in biological structure solution.

The second session of particular personal interest was entitled "New Computational Approaches to Structure Solution and Refinement". This was compromised of several excellent talks detailing a variety of methods to achieve structure solution. **Matt Tucker** described a global optimization process, RMCProfile, which combines data from various types of experiment to model complex structures. A completely different approach described by **Julien Jorda** involved turning the phase problem into a game where human intelligence can be incorporated into the refinement process. Finally, **Briony Yorke** presented a program named HATRIX, which employed the Hadamard matrix as a means of performing time-resolved X-ray crystallography.

The beauty of having such an extensive range of sessions and speakers was that I was able to broaden my knowledge about fields that I would otherwise not have encountered or been exposed to. These included sessions on crystal structure prediction by computational methods, and spectroscopic approaches such as XAFS and XANES in crystallography.

On the whole I thoroughly enjoyed my time in Canada and would like to once again thank the Arnold Beavers Bursary Fund for helping to make my visit possible.

Karim Sutton
University of Oxford



Report on 23rd IUCr General Assembly

The General Assembly took place over three evenings during the IUCr Congress in Montreal (August 5th – 12th 2014). The meeting agenda and papers, and minutes of previous meetings can be found here (www.iucr.org/iucr/governance/ga). Most of the business passed uneventfully in line with the general assembly papers, although there was significant discussion prior to admitting new countries to the IUCr. There were a number of last-minute applications from countries that had been encouraged to pursue crystallographic research through outreach work as part of the International Year of Crystallography. In this context it was the UK delegates' view that, provided they fulfilled the eligibility criteria, then they should be allowed to join irrespective of their level of expertise. Although this may not be a complete list, the following countries were welcomed into the IUCr: Costa Rica, Pakistan, Turkey, Uruguay, Venezuela, Morocco, Cameroon and Algeria, with the decision on Ivory Coast, DR Congo and Malta's applications deferred until the next general assembly. The vote on the location of the 25th IUCr Congress and General Assembly (in 2020) was won by Prague by a large majority. There were also elections for the IUCr Executive Committee. Prof. **Marvin Hackert** was elected President and Prof. **Mike Glazer** was elected Vice President.

David Keen



Education and Outreach Update

FIRSTLY, a huge thank you to all the volunteers who gave up their time to help out at the BCA Education and Outreach events over the last few months. In September the BCA Outreach stand attended the Gravity Fields Festival in Grantham – a week-long festival of science in the birth place of Isaac Newton. The whole town took part with various events from talks to walks and puppet shows to demonstrations, culminating in a lively procession through the town celebrating scientific achievements over the last century. Dr David Price started the crystallographic thread of the event with his talk focussed on Diamond Light Source. The interactive BCA stand entertained school children and shoppers during the week and then hordes of families from toddlers to great-grandparents. Visitors lured in by the lego learnt about diffraction gratings and lattices while operating the replica beamline and producing their own diffraction patterns. They also were able to build their favourite molecules, and make unit cells out of sweets, further emphasising the concept of a crystalline 3D lattice. And if that wasn't enough fun already, visitors were able to learn about the processes of packing and crystal growth by playing with marbles! It was a huge success enabling the celebration of all things crystallographic to be enjoyed in another area of the UK. The event would not have been possible without the enthusiastic and tireless volunteers Lauren Agnew, Sebastian Busch, Simon Coles, Mike Glazer, Lucy Mapp, Alice O'Connor, Jeremiah Tidey and Claire Wilson.



The BCA stand has also been in attendance at the Diamond Open Days, providing infotainment for members of the public before and after their tours of Diamond Light Source. Again, the volunteers **Jonny Brooks-Bartlett, Nick Funnell, Sophie Hesketh, Sam Horell, Nikul Khunti, Euan Pyle, Lucy Saunders, Annabel Taylor, Amber Thompson** and **Philip Welch** made this possible, giving up their time and being so enthusiastic about their science.



There have also been a number of crystallography based interviews and shows in light of the International Year of Crystallography. **Mike Glazer** was interviewed for Lincolnshire radio while at the Gravity Fields Festival, and **Elspeth Garman** featured on BBC Radio 4's 'The Life Scientific Programme' which coincided with the 50th Anniversary of Dorothy Hodgkin's Nobel Prize. Somerville College (Oxford University) also presented 'The Dorothy Hodgkin Symposium' in recognition of her legacy that underpins science today. As part of the International Year of Crystallography, Diamond Light Source produced the film 'The Braggs' Legacy' featuring **Anna Warren**, which celebrates the work and lives of the father and son team and the key achievements in the field in the 100 years since the development of crystallography.

Crystallography has also been on display at the Royal Albert Hall, with the photography exhibition 'Illuminating Atoms' by **Max Alexander**. Max photographed crystallographers with the help of Claire Murray as part of the International Year of Crystallography, incorporating the breadth of the subject, and providing an artist's view point on the integral part it plays in science.

The next BCA Outreach event will be the Big Bang Fair on 11-14 March 2015 at the Birmingham NEC. This will be our 3rd year running at the UK's biggest science and engineering fair for students and families for which there was over 75,000 visitors last year. We will bring the usual Big Bang Fair stand, spanning all aspects of crystallography from growing crystals to solving a crystal structure plus the fundamentals of the theory in between (using sweets and lego!). It is a fantastic opportunity to promote science and crystallography to a large audience, and also to have a lot of fun doing so! As always, we need you to make this event happen. If you are interested in volunteering, or would like more information, please get in contact with us on education@crystallography.org.uk.

If you're interested in learning more, or have an idea for an Outreach event you would like to make a reality, check out our website (learn.crystallography.org.uk), Facebook (British Crystallographic Association Education and Outreach) or Twitter (@Whatsinacrystal) accounts and get in contact with us on education@crystallography.org.uk.

Sam Callear
BCA Education and Outreach Coordinator

Crystallography Fights Ebola

THIS year, each news broadcast seems to carry more depressing and alarming reports about the apparently inexorable spread of the Ebola virus, along with accounts of the frantic efforts to develop a vaccine. However, once again crystallographers have been on the case for well over a decade. The very idea of growing up these extremely dangerous virions and crystallising them is frightening. Instead, efforts have focused on the 7 component viral proteins. Early work sought to obtain the structure of a single protein; more recent studies have examined their modes of association and related them to function. These proteins constitute the RCSB Protein Data Bank Molecule of the Month for October 2014. This article by **David Goodsell**, beautifully illustrated and linked to important structures in the PDB, can be accessed at:

<http://www.rcsb.org/pdb/101/motm.do?momID=178>.

The virus cloaks itself in a membrane purloined from an infected cell. Viral glycoproteins (GPs) emerge from this membrane, giving an appearance like trees emerging from the soil. Covered with carbohydrate chains that help to shield them from the immune system, they change shape once they interact with the surface of a host cell, pulling the viral and host membranes close enough to initiate fusion and start the process of infection. The GP is synthesized as a single-chain precursor and subsequently cleaved into two parts, GP1 and GP2. The latter subunit is responsible for membrane fusion. Its structure was reported in November 1998 by a group with the late Don Wiley of Harvard as corresponding author.

W. Weissenhorn *et al.* (1998) Crystal Structure of the Ebola Virus Membrane Fusion Subunit, GP2, from the Envelope Glycoprotein Ectodomain. *Molecular Cell* **2**, 605–616.

Analysis of the way the glycoprotein interacts with a neutralizing antibody provides an appropriate starting point for attempts at vaccine design. Lee *et al.* did that in 2008. Their findings help to explain why it is so difficult for the human body to combat this virus.

J. E. Lee *et al.* (2008) Structure of the Ebola virus glycoprotein bound to an antibody from a human survivor. *Nature* **454**, 177–182.

Prior to membrane fusion a trimer of GP1 subunits forms a chalice-shaped structure, cradled by GP2 subunits, with the receptor-binding site in the bowl of the chalice. The protective glycan restricts access to the bowl. Antibody KZ52 from a human survivor does not bind there, which would directly block access to the receptor; instead, it binds to the chalice base. Without the crystal structure this site would probably not have appeared to be a primary target for antibody design. Even though receptor binding would still be possible, an antibody at this location, clamping regions of GP2 to GP1, could inhibit the process of fusion.

Immediately below the membrane is a layer formed by matrix proteins, which support it and connect to the nucleocapsid inside. The structure of matrix protein VP40 in monomeric form was determined more than a decade ago. Similarity between the N- and C-terminal domains was noted, along with flexibility in the loop connecting them.

A. Dessen *et al.* (2000) Crystal structure of the matrix protein VP40 from Ebola virus. *EMBO J.* **19**, 4228–4236.

Just how such flexibility could enable this protein to carry out multiple functions was explained last year. VP40 approaches the cell membrane as a butterfly-shaped dimer. There it rearranges to a linear hexamer which is implicated in budding. A third possible structure binds RNA to regulate viral transcription.

Z.A. Bornholdt *et al.* (2013) Structural rearrangement of Ebola virus VP40 begets multiple functions in the virus life cycle. *Cell* **154**, 763–774.

The genome of the virus is protected by nucleoprotein which wraps around the RNA to create a helical structure. Recently the structure of its C-terminal domain has been reported.

P.J. Dziubanska *et al.* (2014) The structure of the C-terminal domain of the Zaire Ebolavirus nucleoprotein. *Acta Crystallogr., Sect.D* **70**, 2420–2429.

Once again, it is multifunctional. As well as its role in assembling the protective nucleocapsid, it is essential for viral transcription and RNA replication. Three additional proteins help with formation of the nucleocapsid structure. Finally, there is an RNA-dependent RNA polymerase which replicates many new copies of the RNA genome.

Sun Tzu's famous advice from The Art of War was to "Know Your Enemy". With regard to the Ebola virus, crystallography is helping us to do just that.

Carl Schwalbe



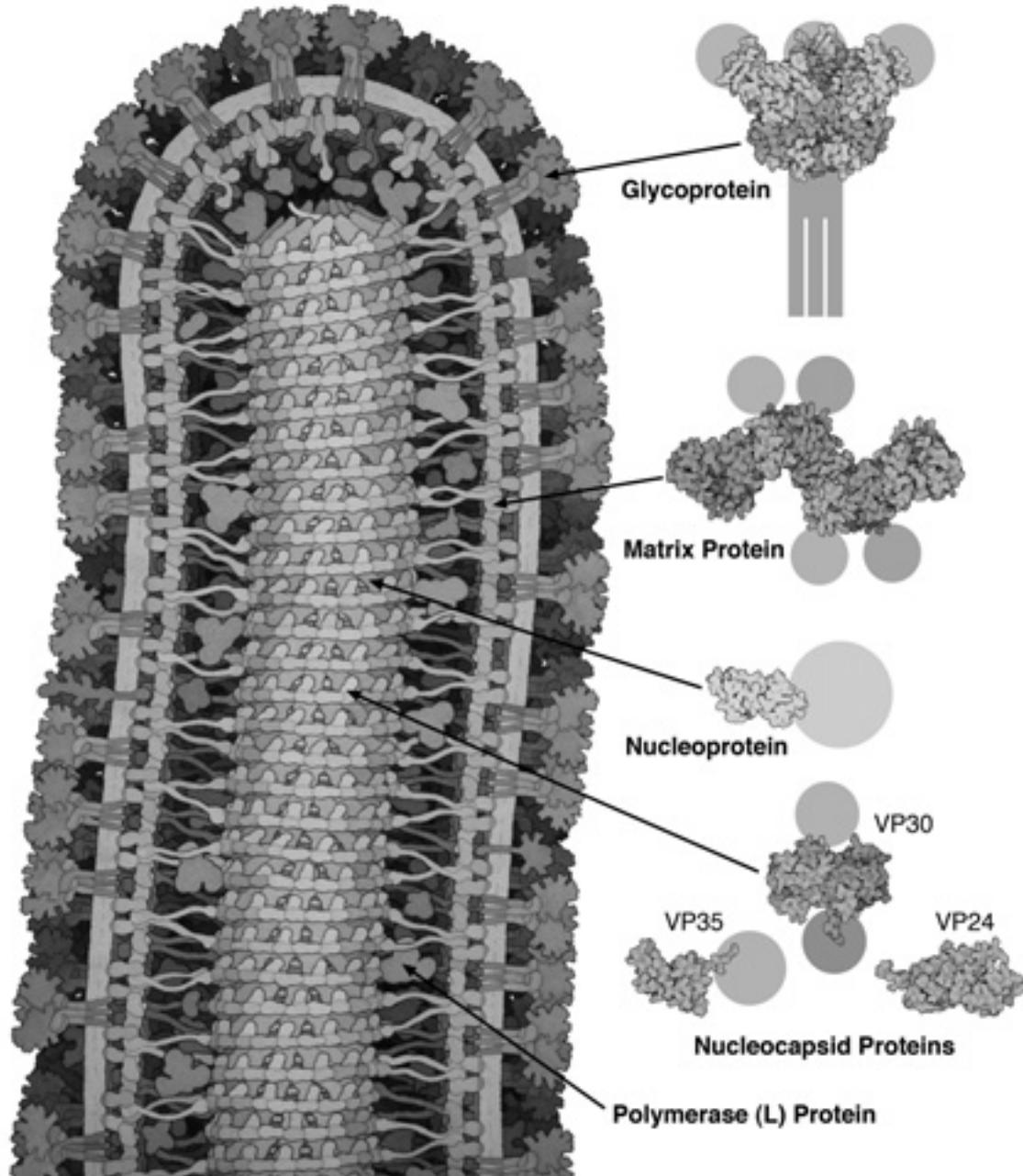


Diagram of the Ebola virus showing the viral proteins and their locations. Reproduced from the RCSB Protein Data Bank Molecule of the Month by permission.

BSG Winter Meeting

THE 2014 BCA-BSG Winter Meeting will take place on the European Photon and Neutron (EPN) Campus, Grenoble, France on 15, 16 and 17 December 2014.

The meeting programme and registration details can be found at <http://www.esrf.eu/home/events/conferences/2014-bca-bsg-winter-meeting.html>

The deadline for registration is 8 December.



Using Crystals to Cure Cancer

Each year, researchers and students at The Institute of Cancer Research are encouraged to hone their science writing skills by competing for a prize – named after Professor **Mal Greaves**, one of the most eminent scientists and skilled communicators at the ICR. Entrants are of course free to write about any area of cancer research. We can be proud that the winner of 2014's *Mal Greaves Science Writing Prize* was Dr **Rohan Bythell-Douglas**, for his piece about crystallography. Reprinted here, it has already been made available on the Web at <http://www.icr.ac.uk/news-features/latest-features/using-crystals-to-cure-cancer>.

ADVOCATES of alternative medicine have long touted the healing effects of strategically placing crystals on parts of your body or around your home. "Ah yes," they say, "if we place some amber around the bedroom, it will absorb all of the negative energy and transform it into healing energy". Crystal healing, as it is known, is nothing more than bunk pseudoscience that does not stand up to scientific inquiry or peer review. However, crystals of another, much smaller variety have been used to develop some very effective cancer treatments. These crystals are very different to the beautiful examples you will see at a holistic healing center or in the geology section of a museum (where they belong). For a start, they are far smaller. Even the largest examples are only just visible to the naked human eye. They are also very fragile, breaking on even the slightest of contact. The vast majority of these crystals don't even come in pretty colours, like jade or sapphire. Instead they are generally clear and colourless. So what is so special about these tiny, fragile, rather plain crystals? These are not crystals of minerals. These are crystals of proteins.

Protein crystals are not a naturally occurring phenomenon. They are produced under highly controlled conditions in a laboratory. Scientists intentionally set out to make a crystal of a specific protein they are researching for a very good reason. A wonderful property of crystals is the way that they interact with light. When light is shone on to a crystal, the light is reflected into a pattern that directly relates to the composition of the crystal. By analysing the pattern of reflected light, scientists can determine what the components within the crystal must look like in order to produce the observed reflection pattern. The method is known as X-ray crystallography because the light used is the same energy as X-rays.

The father-son scientist duo **William Lawrence Bragg** and **William Henry Bragg** won the Nobel prize for discovering this property of crystals. The real power of their discovery is that if you can generate a crystal of the substance you are interested in, you can then determine the structure of the substance you are interested in. So when the crystal is made out of protein, scientists can figure out what the crystallised protein looks like. Knowing the structure of a particular protein can be very useful indeed. Once scientists have identified a certain protein involved in a disease, knowing the structure of that protein makes it far easier to design a drug to bind to the target protein to treat the disease.

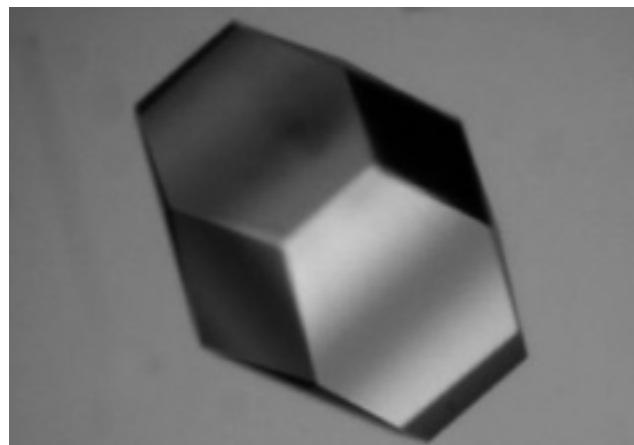


Image of a protein crystal courtesy of Mathias Klode.

Scientists will try to crystallise a protein with a candidate drug to see how the drug binds to the protein and to determine how they can make the drug interact more strongly and specifically. If protein crystals don't already sound science fiction enough, scientists often use a type of particle accelerator called a synchrotron to produce the specific type of high-energy light they need for this experiment. Why don't they just use a microscope to look directly at the protein without worrying about making a crystal in the first place? This method involving crystal-reflected light patterns provides a far higher resolution structure of the protein than even the most advanced microscopes and has done so for the last 50 years!

A brilliant example of a cancer-causing protein successfully targeted by this crystal-mediated process is the Bcr-Abl fusion protein. Bcr and Abl are two different proteins that are separate from one another in healthy cells. In some people, there is a rare genetic event that causes the two proteins to fuse together to form the Bcr-Abl fusion protein. When these two proteins are fused together, the cell loses the ability to regulate the activity of these proteins, which causes chronic myeloid leukemia.

Armed with this knowledge, scientists targeted the Bcr-Abl fusion protein for drug design. Researchers carried out an iterative drug design process, where they generated crystals of the Bcr-Abl fusion protein that had been incubated with candidate drug-like compounds. After much research carefully analysing the structure of the protein in the presence of

various drug-like compounds and further optimisation, the project eventually yielded the drug imatinib (marketed as Gleevec or Gleevec).

Clinical trials demonstrated that imatinib was an effective drug against chronic myeloid leukaemia caused by the Bcr-Abl fusion protein. Some 98% of patients showed complete haematologic response after five years of imatinib therapy. This essentially means that their white blood cell count had returned to healthy, non-cancerous levels. Staggeringly, imatinib increased the survival rate of patients with chronic myeloid leukemia from 30% to 89% five years post diagnosis. Such was the success of the drug that imatinib made the cover of Time magazine in 2001 as the 'magic bullet' to cure this type of cancer. A life-saving discovery had been made through the use of protein crystals.

Protein crystals have played an essential role in the development of several other drugs for the treatment of numerous diseases, including swine flu, HIV and hepatitis C. The development of imatinib to treat chronic myeloid leukemia is a brilliant example of how we really can use crystals to cure cancer.

References

Druker, B. J., et al. Five-year follow-up of patients receiving imatinib for chronic myeloid leukemia, *New England Journal of Medicine* 355, 2408–2417 (2006).

Dr Frank Allen FRSC CChem 1944-2014



IT is with great regret we announce that Frank Allen died, 10th November, aged 70. Frank joined the Chemical Crystallography Group at the University of Cambridge in 1970 and played a pivotal role in the establishment of the Cambridge Structural Database. He went on to become the Scientific Director and then the Executive Director of the Cambridge Crystallographic Data Centre.

Following his retirement in 2008, Frank remained with the CCDC as an Emeritus Research Fellow, enabling him to continue to indulge his passion for structural chemistry.

Frank's research involved collaboration with many scientists around the world, resulting in over 200 papers. He was also a wonderful teacher, supervising more than 20 doctoral students and introducing many more to structural chemistry through workshops over many years.

His contributions to other influential organisations, his vigorous editorship of *Acta Crystallographica*, the numerous conferences he organised and presentations he made meant Frank was known to and respected by crystallographers the world over.

Frank has long been a leading figure in international crystallography, and was a wonderful colleague, becoming a friend to all those who worked with him. He will be sadly missed.

(From the CCDC website) A full obituary will follow in a future issue.

A Crystallographic Dinosaur

by Stephen Wallwork



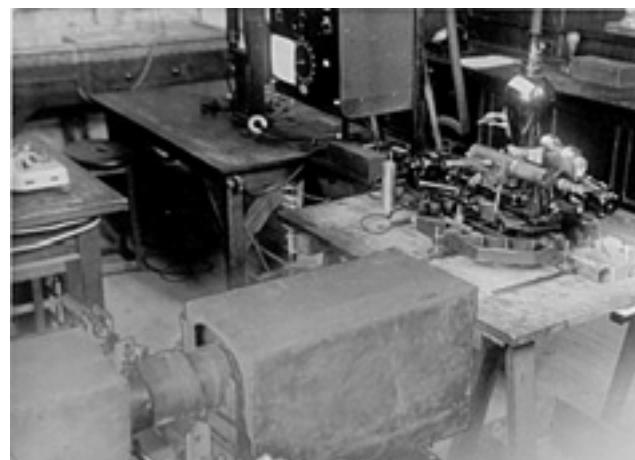
Stephen Wallwork

NOW 89 years of age, I have realised that I am one of only a few survivors of an age that present-day crystallographers probably know little about. So this is an account of what crystallography was like when I first became involved in it, before there were computers and diffractometers.

I first encountered crystallography in 1943 when I became an undergraduate at Brasenose College, Oxford. This was only thirty years after the Braggs had started crystal structure determinations. The Oxford chemistry course consisted of three taught years for Part 1 and a research year as Part 2. Crystallography lectures were available during Part 1, taught almost entirely by **H M Powell**, known to everybody as Tiny because of his small stature. Most of the undergraduates in my year found the course to be rather difficult and stopped attending after a few weeks. I had registered to take an additional subsidiary course in practical crystallography and I found that this 'hands-on' experience made the lecture course much more understandable. What is more, since the Oxford crystallography section originated as part of the mineralogy department, the lecture course included optical crystallography and I much enjoyed the lecture illustrations of this aspect, demonstrated with the aid of a projection polarising microscope. The practical course also contained elements of classical crystallography, such as the use of an optical goniometer to measure angles between crystal faces.

This was followed by the plotting of the results as a stereographic projection to reveal the symmetry and hence the crystal system. This was complemented by the use of the polarising microscope to study optical properties of crystals. Only later in the course did one learn how to interpret X-ray oscillation photographs and eventually Weissenberg photographs.

I don't think we actually took any X-ray photographs as part of the practical course over three years, but that followed in the Part 2 research year, 1946/7. Though there was a sealed X-ray tube in the X-ray room, there was still a continuously pumped tube that had been constructed by Powell. If only one of its two X-ray beams was in use, the second port was covered by putting in place a piece of lead bent to sit on top of the horizontal tube. One had to make sure that one was not exposed to radiation during this process though one did get an occasional electric shock.



Oxford X-ray room 1949.

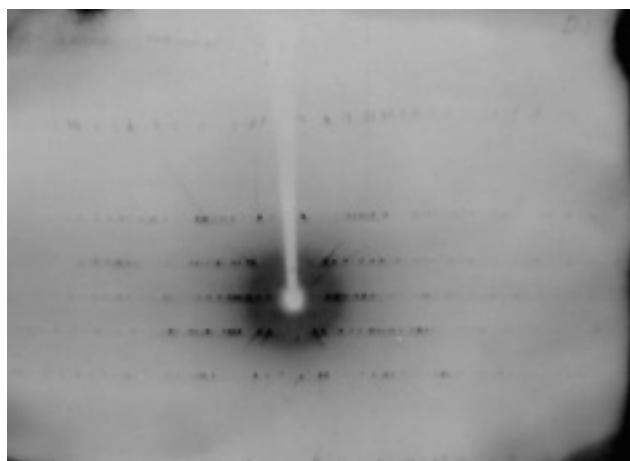
It was still some years prior to the invention of the first diffractometer, of course, so all X-ray data were collected photographically. Intensities of spots thus photographed were estimated by eye, by comparison with a strip of spots of increasing blackness. This strip was preferably prepared from the same crystal that was being measured by exposing one of its spots for successive multiples of an initial number of seconds. Needless to say, this matching process was a rather stressful, time consuming, and not particularly accurate procedure and was also a strain on the eyes.

Structure solution was carried out by proposing a trial structure, sometimes based on interpretation of Patterson syntheses, then calculating structure factors for this structure using a desk adding machine and comparing them with the observed structure factors derived from the observed intensities. If the two compared reasonably well, one could proceed to refinement. This consisted of a cycle of Fourier syntheses calculated using the derived approximate phases

and the observed structure factors to obtain improved atomic positions, followed by an improved calculation of structure factors. The cycle was repeated until there was no further improvement. Because of the time and effort involved in doing these calculations by hand, even though the Fourier syntheses were aided by Beevers-Lipson strips, it was common practice to calculate only for two projections of the structure, using two of $hk0$, $h0l$, $0kl$ structure factors, rather than for a three-dimensional structure using all hkl reflections. One round of structure factor and Fourier calculations would take anything from a day to a week, even for a projection. Direct methods of structure solution were about to be introduced but these were also tedious to apply by hand. (David Sayre derived his well-known structure factor relationships while working in Oxford during my doctoral research years there, 1946-1949.)

I was appointed to the academic staff of the Chemistry Department at the University of Nottingham in 1949 and, needless to say, as soon as the acquisition of a computer was mooted there, I was one of the enthusiastic supporters. When one was eventually installed it was only operated by professionals, took up the whole of a fairly large room, and had a storage capacity a tiny fraction of that in today's mobile phones.

The slower pace of crystallographic research meant that there was more encouragement to try new ideas. In my case, Tiny Powell suggested that I should calculate the Fourier transform for the quinol molecule and project the reciprocal lattice of its alpha crystal form, then under investigation, onto the transform, as a way of calculating structure factors. It worked in principle but was far too approximate for that particular structure. Much more successful was my use of a photometer designed to measure the blackness of lines in spectra, adapted to measure the spots on the X-ray photographs. This eliminated the subjective nature of eye comparisons. I also constructed a cooling system – first, one to fit on an oscillation camera and then, later, one to fit a Weissenberg camera. Such diversions were a welcome relief from punching numbers on an adding machine all day.



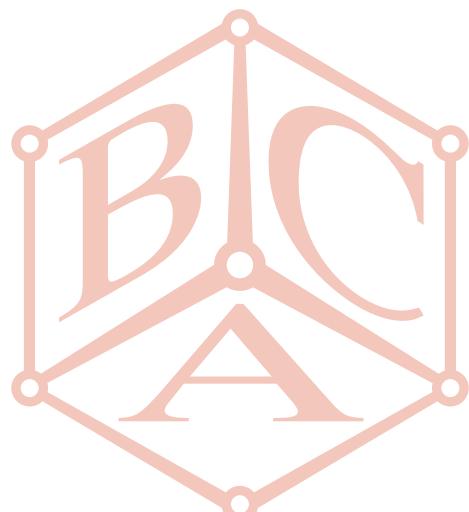
Quinol oscillation.

During the relatively short time over which I have been involved in crystallographic research, the subject has evolved tremendously. Diffractometers have replaced the painstaking measurement of photographic intensities. Structure solution is routinely done by direct, dual space or charge flipping methods, and refinement is by least-squares methods, all

carried out automatically on computers. This brings about a fantastic increase in productivity but I wonder whether there is still the sense of achievement that resulted from pitting one's skills and patience against nature in solving and refining structures the old-fashioned way?



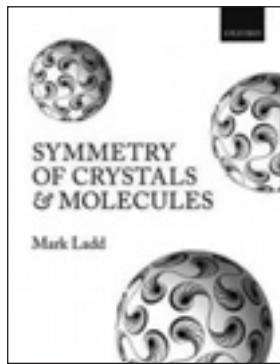
Nottingham lab 1950.



Symmetry of Crystals and Molecules

by Mark Ladd

Oxford University Press 2014, 433 + xxi pages, 8 colour plates, £55.00 (hardback), ISBN 978-0-19-967088-8.



FORMERLY Head of Chemical Physics at the University of Surrey, Dr Mark Ladd's latest book distils his considerable expertise gained over many years of teaching crystallography to university students, both at undergraduate and postgraduate levels. There are numerous illustrations, some appearing as stereoscopic pairs. At the end of each chapter, one finds comprehensive lists of

references to the scientific literature, both historic and recent; and the various topics are supported by thirteen appendices. He has set numerous problems to do and, most helpfully for the student, there are 31 pages of tutorial solutions at the end of the book. Computer programs, freely available from the publisher's website

www.oup.co.uk/companion/ladd, add to the fine didactic quality of this textbook.

It starts with a handy list of physical data and notation. Chapter 1 (12 pages) is a gentle introduction to symmetry, appealing to everyday objects for illustrations. Chapter 2 (50 pages) on the geometry of crystals and molecules, sets the scene with the necessary equipment including such topics as Miller indices, stereographic projection, axial ratios, bond distances and bond angles, errors, orbitals and crystal packing. To my mind, I think that some of the geometrical results could have been more elegantly derived using vectors, especially by use of the powerful but simple scalar product and vector product. (Indeed, there is an appendix on these two products.)

Point group symmetry is the major topic of Chapter 3 (56 pages). Group theory will come later (in Chapter 7): even so, I think it would have been helpful to have outlined the meaning of the word 'group' at this stage, or at least to have provided a forward reference to page 240. In Figure 3.12, I found the placing of the headings and the grouping of the stereograms of the 32 crystallographic point groups rather confusing. The caption says that they are arranged by crystal system and Laue class; but at this stage, 'Laue class' has yet to be defined. Understandably, the reader has to read on to the next chapter (page 139) for an explanation of why, among all possible rotational symmetries, they exist in crystals in only 1, 2, 3, 4 and 6-fold varieties. The chapter continues with interesting sections on the role of point group symmetry in determining some of the physical properties of crystals and molecules; examples of symmetrical chemical species; the Hermann-Mauguin and Schoenflies notations; matrix representations of symmetry operators; quasicrystals and icosahedral symmetry.

Lattices (Chapter 4, 30 pages) are logically constructed in one, two and three dimensions; and the reciprocal lattice is introduced. Also treated are the law of rational intercepts; reticular density; and lattice transformations. This chapter prepares the reader for the next one: Chapter 5 (69 pages) on space groups. This too builds up to three dimensions by considering one and two dimensions first. Screw axes and glide planes are described there; and many space-group diagrams have been reproduced from the *International Tables for Crystallography* Volume A together with instructive explanations. Examples given of crystal structures include sodium chloride, the alums, copper oxide, and spinel and inverse spinel structures. Black-and-white symmetry and colour symmetry are also mentioned.

X-ray diffraction (Chapter 6, 21 pages) is briefly described, together with the reciprocal lattice and Ewald construction. Geometrical structure factors are calculated here for various space groups. Group theory itself is treated in Chapter 7 (44 pages); and deals with describing representations and constructing character tables, using matrix algebra going well beyond the A-level mathematics mentioned as a pre-requisite on the back cover of the book. Applications of group theory are given in the 50 pages of Chapter 8. Here Monte Carlo and molecular dynamics techniques are outlined; and the symmetries and molecular orbital energies of various molecules are described, featuring particularly water, methane, benzene, and some transition metal coordination compounds. Examples of infrared and Raman spectra are given in the section on vibrational studies; and this is followed by sections on group theory and point groups; group theory and space groups; and factor groups.

The various computer-assisted studies are listed in the short Chapter 9 (4 pages). The appendices (comprising 54 pages) have the following titles: Stereoviews and crystal models; Analytical geometry of direction cosines; Vectors and matrices; Stereographic projection of a circle is a circle; Best-fit plane; General rotation matrices; Trigonometric identities; Spherical polar coordinates; The gamma function; Point group character tables and related data; Linear, unitary and projection operators; Vanishing integrals; and Affine groups.

Like a high-quality diamond, this book has some imperfections. There are a few typographical errors. In Example 2.4, the value of R given for $r = 60$ pm appears to be a minimum rather than a maximum. Figure 3.41(d) shows a pentagonal (or Platonic) dodecahedron – not a rhombic dodecahedron. The final line in Section 7.4.1(a) should read $AE = A$ (not E). The lower limits on the integrals of Example 7.3 should be $-\pi$. The last sentence of appendix section A1.2 belongs in section A1.1. In examples of vectors (A3.2), although $30^\circ N$ has magnitude and direction, it is not a vector. Angular displacements do not even commute: α followed by β is not the same as β followed by α .

This well-produced book will appeal more to the budding structural chemist than to students of physics or mineralogy. Of interest to the solid-state physicist are the defects in crystals, their various symmetries and how they may greatly modify some physical properties of materials, but these are not covered. It is nevertheless a worthy volume to be added to all those excellent books published during the International Year of Crystallography.

Moreton Moore
Royal Holloway University of London

Meetings of interest

FURTHER information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

10-11 December 2014

SC2014. Novel SuperConductors and Synchrotron Radiation: state of the art and perspectives, Trieste, Italy.
www.elettra.trieste.it/Conferences/2014/SCSR

10-17 December 2014

Diamond-CCP4 Data Collection and Analysis workshop.
<http://www.diamond.ac.uk/Home/Events/2014/Diamond-CCP4-Data-Collection-and-Analysis-workshop.html>

11-12 December 2014

International Workshop on Advances in X-ray Imaging, Trieste, Italy.
www.elettra.trieste.it/Conferences/2014/wsimaging/

15-17 December 2014

BCA-BSG Winter Meeting, Grenoble, France.
<http://www.esrf.eu/home/events/conferences/2014-bca-bsg-winter-meeting.html>

15-19 December 2014

Structural Biology: Using Synchrotron Radiation to Visualize Biological Molecules, Trieste, Italy.
http://agenda5.ictp.trieste.it/full_display.php?id=a13194

7-9 January 2015

CCP4 Study Weekend, "Advances in Experimental Phasing", Nottingham.
http://www.cse.scitech.ac.uk/events/CCP4_2015/Register.asp

12-13 January 2015

Future Muon Sources, Huddersfield.
<http://wwwisis2.isis.rl.ac.uk/useroffice/MuonSources/Register.asp>

14-16 January 2015

BioXFEL. 2nd International Conference, Ponce, Puerto Rico.
<https://www.bioxfel.org/events/details/6>

18-23 January 2015

6th MaNEP Winter School, "Shedding light on correlated electrons, Saas-Fee, Switzerland.
www.manep.ch/saasfee15/

22-23 January 2015

10th SOLEIL Users' Meeting, Saint Aubin, France.
www.synchrotron-soleil.fr/Workshops/2015/SUM2015

26-27 January 2015

BESSYII – From PICO to FEMTO. Workshop on time-resolved studies at BESSY II. Berlin-Adlershof, Germany.
www.helmholtz-berlin.de/user/workshops/from-pico-to-femto/index_en.html

28-30 January 2015

2015 European XFEL Users' Meeting and Satellite Meetings, DESY, Hamburg, Germany.
www.xfel.eu/events/users_meetings/2015_users_meeting/

29-30 January 2015

ISIS Molecular Spectroscopy Scence Meeting, Abingdon.
<http://wwwisis2.isis.rl.ac.uk/useroffice/MoleSpecUGM2015/Register.asp>

7-11 February 2015

59th Biophysical Society, Baltimore, MD, USA.
www.biophysics.org/2015meeting/Main/tabid/4837/Default.aspx

15-18 February 2015

4th Banff Meeting on Structural Dynamics, Banff, AB, Canada.
www.sun.ac.za/Banff

23 February – 6 March 2015

46th IFF Spring School 2015 on Functional Soft Matter, Jülich, Germany.
springschool@fz-juelich.de

26 February – 6 March 2015

35th Berlin School on Neutron Scattering, Helmholtz Zentrum, Berlin, Germany.
www.helmholtz-berlin.de/events/neutronschool/index_de.html

28 February – 3 March 2015

5th Winter School on Soft X-rays in Macromolecular Crystallography, Athens, GA, USA.

1 March – 1 April 2015

HERCULES 2015 – European School, Grenoble, France.
<http://hercules-school.eu/>

2-6 March 2015

7th ILL Annual FullProf School, Grenoble, France.
www.ill.eu/FPSchool2015/

9-13 March 2015

Hybrid Materials 2015, Sitges (near Barcelona), Spain.
www.hybridmaterialsconference.com/

16-19 March 2015

23rd Annual Conference of the German Crystallographic Society, Göttingen, Germany.
www.dgk-conference.de/organizational-matters/goettingen/

21-29 March 2015

XV Intensive Teaching School in X-ray Structure Analysis, Durham.
<http://community.dur.ac.uk/durham.x-ray-school/>

29 March – 2 April 2015

Microscopy of Semiconducting Materials (MSM-XIX), Cambridge.

<http://msm2015.iopconfs.org/home>

30 March – 2 April 2015

BCA Spring Meeting, York.

www.crystallography.org.uk

30 March – 2 April 2015

Interdisciplinary Surface Science Conference (ISSC-20), Birmingham.

<http://issc-20.iopconfs.org/home>

30 March – 1 April 2015

Nucleation – a Transition State to the Directed Assembly of Materials. Faraday Discussion. Leeds.

www.rsc.org/ConferencesAndEvents/RSCConference/s/FD/Nucleation-FD2015/index.asp

13-15 April 2015

Corrosion Chemistry, Faraday Discussion. London.

www.rsc.org/ConferencesAndEvents/RSCConferences/FD/Corrosion-FD2015/index.asp

19-24 April 2015

56th Experimental Nuclear Magnetic Resonance Conference, Pacific Grove, CA, USA.

www.enc-conference.org/

20-22 April 2015

Nanoparticle Synthesis and Assembly. Faraday Discussion. Chicago, IL, USA.

<http://www.rsc.org/ConferencesAndEvents/RSCConferences/FD/Nanoparticle-FD2015/index.asp>

20-22 May 2015

Fourth International Symposium Frontiers in Polymer Science, Riva del Garda, Italy.

www.frontiersinpolymerscience.com/index.html

5-14 June 2015

Engineering Crystallography: from Molecule to Crystal to Functional Form. 48th Erice Course, Erice, Italy.

www.crystalerice.org/Erice2015/2015.htm

7-12 June 2015

Computational Aspects – Biomolecular NMR: Exploring the Frontiers of NMR, Computations and Complementary Biophysical Methods. Gordon Research Conference, Lucca, Italy.

www.grc.org/programs.aspx?id=14571

7-20 June 2015

The Zürich School of Crystallography: bring your own crystals, Zürich, Switzerland.

www.chem.uzh.ch/linden/zsc/

22-24 June 2015

Mesoscopic & Condensed Matter Physics, Boston, MA, USA.

<http://condensedmatterphysics.conferenceseries.com/>

28 June – 2 July 2015

ZMPc 2015. International Symposium on Zeolites and MicroPorous Crystals, Sapporo, Japan.

www.zmpc.org/

6-10 July 2015

SRI2015. 12th International Conference on Synchrotron Radiation Instrumentation, New York, NY, USA.

www.bnl.gov/sri2015/

18-22 July 2015

ESBA2015. 10th European Biophysics Congress, Dresden, Germany.

www.ebsa2015.com

20-23 July 2015

12th International Conference on Materials Chemistry (MC12), York.

www.rsc.org/ConferencesAndEvents/RSCConferences/MC12/index.asp

25-29 July 2015

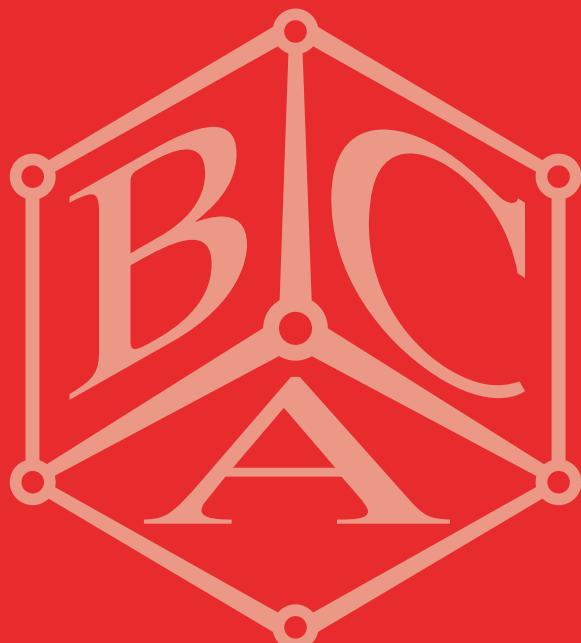
ACA2015. American Crystallographic Association Annual Meeting, Philadelphia, PA, USA.

www.amercrystalassn.org/

23-28 August 2015

ECM29. The 29th European Crystallographic Meeting, Rovinj, Croatia.

<http://ecm29.ecanews.org/>





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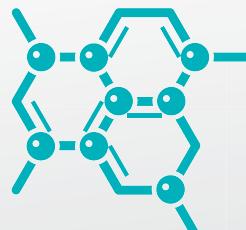
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